Predicting asymmetric phospholipid microstructures in solutions

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Fig. S1

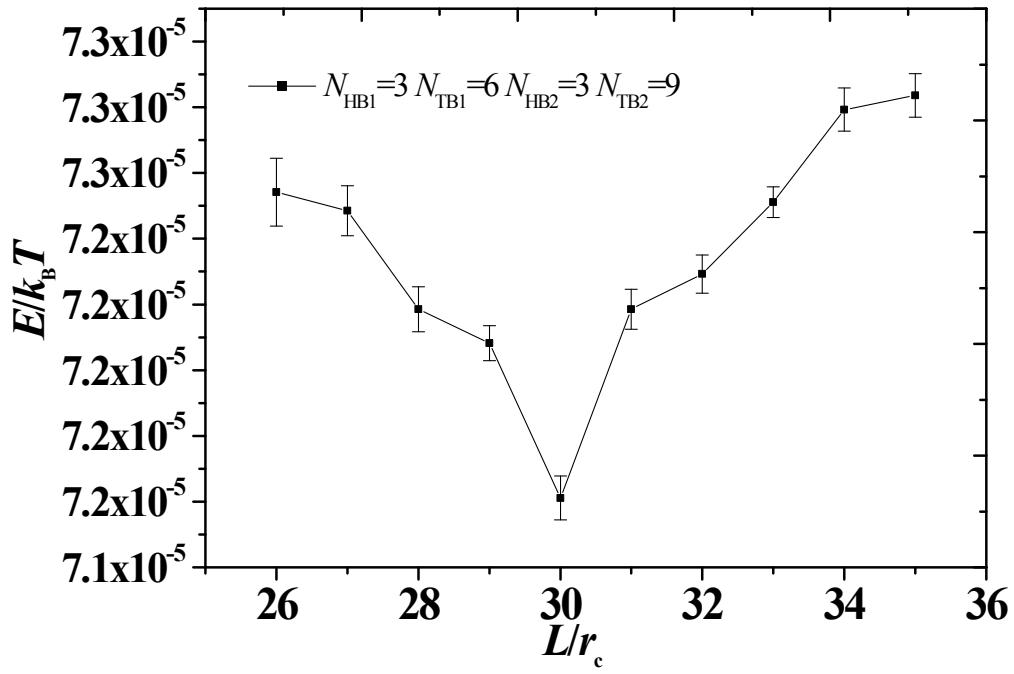

Fig.S1 The average energy of molecule as function of box size L. The phospholipid with the parameter of $N_{HB1}=3$, $N_{HB2}=3$, $N_{TB1}=6$, and $N_{TB2}=9$.

Fig.S2

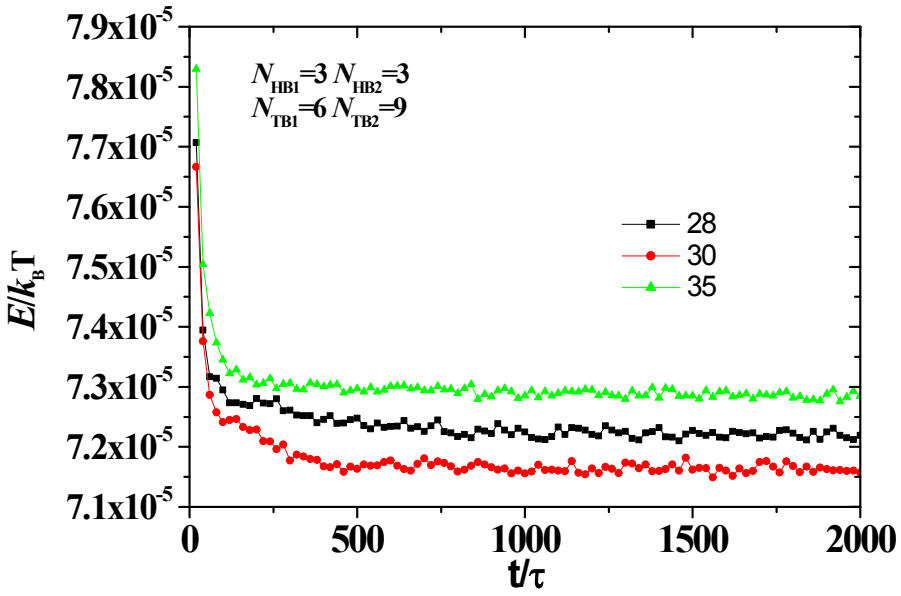

Fig.S2 The average energy of molecule as function of time step. The phospholipid with the parameter of $N_{HB1}=3$, $N_{HB2}=3$, $N_{TB1}=6$, and $N_{TB2}=9$. The box sizes L are set to be $L=28r_c$, $30r_c$ and $35r_c$.

Fig.S3

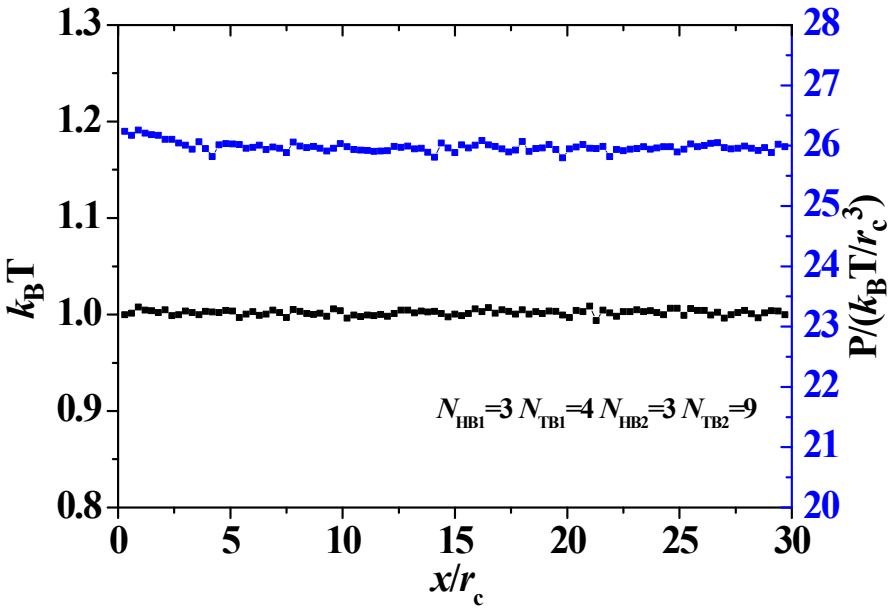

Fig.S3 The local pressure *P* and temperature *T* as functions of *x*.

Fig.S4

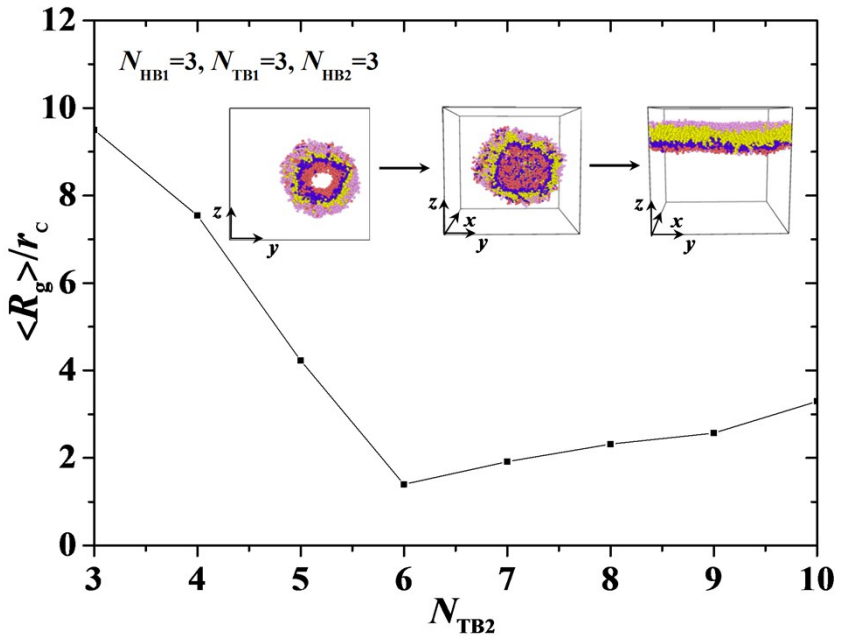

Fig.S4 The average of radius of gyration as a function of N_{TB2}, with $N_{HB1}=3$, $N_{TB1}=3$, and $N_{HB2}=3$ The corresponding asymmetric structures are also inserted.